

# Argonne National Laboratory

CALCULATION OF  $dE/dx$  AND  
ENERGY LOSS DISTRIBUTIONS IN  
SPHERICAL CAVITIES FOR  
MONOENERGETIC NEUTRON FIELDS

by

Robert F. Dvorak

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Industrial Hygiene and Safety Division

May 1968





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ABSTRACT

A computer program has been prepared that calculates the average  $dE/dx$  and energy loss for events occurring in a spherical cavity due to incident monoenergetic neutrons. No assumptions are made as to distribution of path lengths. The particle paths are traced and a range-energy equation is used to calculate the cavity energy loss and average  $dE/dx$  for each event.

The distribution in pulse height for events having the same average  $dE/dx$  is shown to be a function of both average  $dE/dx$  and the neutron energy, and to deviate from the commonly postulated triangular distribution at neutron energies below 1 MeV for a cavity with a diameter of  $2.08 \mu\text{m}$ . Pulse-height distributions and dose distributions in average  $dE/dx$  for several energies have been computed. From the pulse-height distributions, LET distributions were calculated by the Rossi-Rosenzweig technique and compared with the computed average  $dE/dx$  distribution.

The weighting factor relating energy loss and deposited dose equivalent for an event, as used with the survey instrument proposed by Baum, was also computed. It is shown to be dependent on the neutron energy, and to vary by as much as a factor of three in a region of heavy-event population.

INTRODUCTION

A device for the measurement of dose as a function of specific ionization was introduced by Rossi and Rosenzweig in 1955.<sup>1</sup> This device, which is generally called the Rossi LET Counter, has been utilized by a small number of investigators<sup>2-5</sup> to determine dose and dose equivalent distributions in mixed radiation fields.

The technique originally presented for evaluation of data<sup>1</sup> was later clarified in an unpublished memorandum by Rosenzweig in May 1960, and serves as the basis for contemporary work with the instrument.





The following assumptions are critical to the analysis:

1. A spherical cavity is surrounded by a tissue-like wall and irradiated in an isotropic neutron field.
2. Neutron attenuation in the wall is negligible.
3. The recoil particles generated have constant  $dE/dx$  from birth to the point at which they leave the cavity.
4. The range of recoil particles is sufficiently great that it always traverses the cavity.
5. Contributions to the spectrum due to recoils originating in the cavity are negligibly small.

None of these assumptions are strictly correct if real recoil particles are considered. The assumptions approach reality as either the neutron energy is increased or the cavity size is decreased. These limitations were recognized by Caswell<sup>6</sup> and by Lawson and Watt.<sup>7</sup> This being the case, the questions that immediately arise are how great is the error in the conventional Rossi analysis, and, if the error is significant, is there a more accurate means to transform the energy-loss distributions measured by the proportional counter into the corresponding LET distributions. The work presented here explores these questions.

## DESCRIPTION

To achieve these ends, a computer program was prepared for the Argonne CDC 3600 computer. The program simulates the recoil processes occurring in a spherical cavity within a tissue-like spherical medium of finite dimensions that results from irradiation by unit isotropic fluence of neutrons. The computation begins with the isotropic distribution of proton or carbon recoils, and by programmed samples over all possible initial energies, wall depths, and angles of emission, synthesizes the actual spectra resulting from cavity traversals.

Analytical expressions for energy as a function of particle residual range were necessary for use in the computation. Basic data for  $dE/dx$  versus energy for protons were taken from published work by Snyder and Neufeld,<sup>8</sup> Janni,<sup>9</sup> the National Research Council,<sup>10</sup> Snyder,<sup>11</sup> and Turner.<sup>12</sup> The basic data for carbon ions, which are not particularly accurate, were taken from Snyder and Neufeld,<sup>8</sup> Steward and Wallace,<sup>13</sup> and Snyder.<sup>11</sup>

The various data were combined to develop "reasonable"  $dE/dx$  versus energy curves for each particle. Analytical expressions for  $dx/dE$  versus energy were then prepared using a least-squares data-fitting program. The expressions for residual range as a function of



energy were obtained by integration of the  $dx/dE$  versus energy functions. Finally, data taken from the residual range versus energy function were refitted to give the desired energy versus residual range functions.

Having developed these conventional energy-related functions, we developed a corresponding set of damage functions. If we define

$$\text{Rate of Damage} = \frac{dB(x)}{dx} = Q\left(\frac{dE}{dx}\right) \frac{dE}{dx} \quad (\text{MeV-cm}^2/\text{g})$$

where  $Q\left(\frac{dE}{dx}\right)$  is the Quality Factor, we can define

$$\text{Residual Damage} = B(x) = \int_x^{x=0} Q\left(\frac{dE}{dx}\right) \frac{dE}{dx} dx \quad (\text{MeV}).$$

The analytical expressions for damage as a function of residual particle range were prepared for both protons and carbon ions.

Calculation of the parameters for ionizing events entering the cavity proceeds was based on the following assumptions:

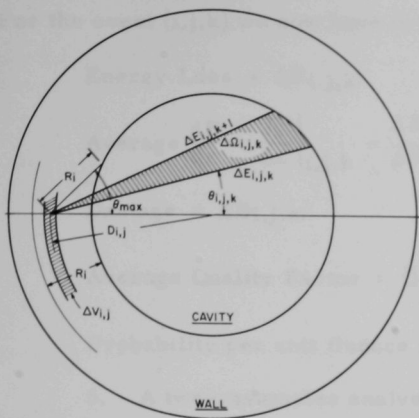
1. Since the neutron fluence is isotropic, the recoils are also isotropically distributed in direction.
2. In each direction, all recoil energies between zero and the allowed maximum are equally probable.
3. The recoils travel in straight lines.
4. No neutron attenuation occurs in the cavity wall, and each event is the result of a first collision.
5. The cavity diameter is large compared to the diameter of the ionized column, so that, effectively, the  $dE/dx$  energy loss remains within the cavity boundary.
6. All energy losses are through the mechanism of ionization.

For recoils originating in the wall, the computation proceeds as follows:

1. The maximum recoil energy is determined, and I equally incremented energy groups are established between zero and maximum energy. The midenergy  $E_i$  and the corresponding particle range  $R_i$  are determined for each group.







235-1505

Fig. 1. Representation in Two Dimensions of the Geometric Relationships Used in Computing Traversal Probabilities and Path Lengths for Recoils Originating in the Wall Volume

defined by  $(\theta_{\max})_{i,j}$  is divided into  $K$  bounded by  $\theta_{i,j,k}$  and  $\theta_{i,j,k+1}$ , where

$$\theta_{i,j,k} = \frac{k(\theta_{\max})_{i,j}}{K}.$$

The fractional solid angle  $\Omega_{i,j,k}$  for the conical shell of revolution defined by  $\theta_{i,j,k}$  and  $\theta_{i,j,k+1}$  is determined.

4. Having calculated  $\theta_{i,j,k}$  and  $D_{i,j}$ , and using input data for cavity density, wall density, and cavity radius, it is a simple geometrical calculation to determine the path length for the recoil in the wall and maximum possible path length in the cavity. Starting with  $R_i$ , the range of the recoil, the residual range at the cavity interface on entry and exit is determined. Borrowing Caswell's<sup>6</sup> terminology, the track length in the cavity  $\Delta X_{i,j,k}$  is equal to the difference in residual ranges for "crossers," and equal to entry residual range for "stoppers." From the range-energy equations, the energy of the recoil at the entry and exit cavity interfaces is calculated. The energy loss in the cavity  $\Delta E_{i,j,k}$  is equal to the difference in energies for "crossers" and to the entry energy for "stoppers." Continuing, and using the residual damage-range equations,  $\Delta B_{i,j,k}$  is calculated. Finally, the probability per unit neutron fluence of a recoil of energy  $E_i$  originating in the shell at radius  $D_{i,j}$  and traveling in the conical shell between  $\theta_{i,j,k}$  and  $\theta_{i,j,k+1}$  is calculated as

$$P_{i,j,k} = \sum_{i,j} \Omega_{i,j,k}.$$

2. For each  $E_i$ , and measuring outward from the wall-cavity interface, the recoil-contributing wall volume between zero and  $R_i$  is divided into  $J$  concentric spherical shells of thickness  $R_i/J$  with mid-radius  $D_{i,j}$  (see Fig. 1). Using input values of wall density and neutron macroscopic elastic cross section, and calculating the shell volume  $V_{i,j}$ , the probability per unit fluence  $\Sigma_{i,j}$  of a recoil of energy  $E_i$  being generated in the shell volume  $V_{i,j}$  is determined.

3. For each  $E_i$  and each shell radius  $D_{i,j}$ , the maximum angle  $\theta_{\max}$  is calculated on which a recoil can travel and either graze or just reach the cavity interface. The cone of revolution conical shells of revolution, each



For the event  $(i,j,k)$  we now have or can compute the following information:

$$\text{Energy Loss} = \Delta E_{i,j,k};$$

$$\text{Average } \frac{dE}{dx} = \left. \frac{d\bar{E}}{dx} \right|_{i,j,k} = \frac{\Delta E_{i,j,k}}{\Delta X_{i,j,k}};$$

$$\text{Damage} = \Delta B_{i,j,k};$$

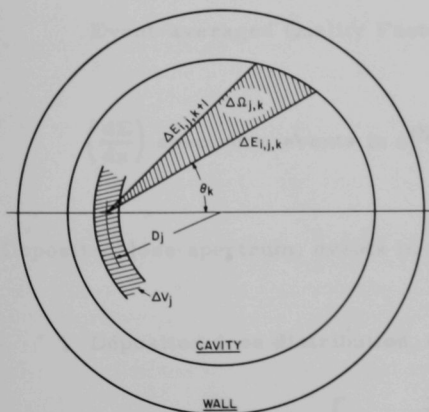
$$\text{Average Quality Factor} = \bar{Q}_{i,j,k} = \frac{\Delta B_{i,j,k}}{\Delta E_{i,j,k}};$$

$$\text{Probability per unit fluence of event} = P_{i,j,k}.$$

5. A two-parameter analysis is now performed in the following manner:

The first parameter is placed along what we shall refer to as the X axis and in this program is always  $\Delta E_{i,j,k}$ . The second parameter, along the Y axis, is selectable as either  $(dE/dx)_{i,j,k}$ ,  $\Delta B_{i,j,k}$ , or  $\bar{Q}_{i,j,k}$ . Each axis is dimensioned appropriately and into a maximum of 100 equal increments or "channels."

Corresponding to  $P_{i,j,k}$  we have, according to one option, a range of  $\Delta E$  between  $\Delta E_{i,j,k}$  and  $\Delta E_{i,j,k+1}$ , and a range of  $dE/dx$  between  $(dE/dx)_{i,j,k}$  and  $(dE/dx)_{i,j,k+1}$ . If the area in the X-Y plane defined by these values encompasses  $mn$  channels, then the increment  $P_{i,j,k}/mn$  is added to each of the involved channels. Effectively, event probability is accumulated in the Z axis direction as the analysis is performed for each of the  $i, j, k$  events.



235-1506

Fig. 2. Representation in Two Dimensions of the Geometric Relationships Used in Computing Traversal Probabilities and Path Lengths for Recoils Originating in the Cavity

The calculation of recoils originating in the cavity is next undertaken and proceeds in an identical manner. Referring to Fig. 2, the important differences are that  $\theta$  and  $D$  are independent of proton energy  $E_i$ , the concentric shells have radii  $D_i$  between zero and the cavity interface radius, and  $\theta_{\max}$  is always  $180^\circ$ . The equations for calculation of the geometric path length at angle  $\theta_{j,k}$  are, of course, different, and the proton enters the energy-loss calculation with energy  $E_i$ .





To include carbon recoils in the spectrum, it is necessary only to repeat the above calculations with residual range-energy and residual energy-residual damage equations that are calculated for carbon ions.

After the two-parameter analysis has been performed and committed to the computer memory, it is possible to calculate easily and quickly a number of very useful summations, some of which are indicated below:

$$\text{Number of Events} = \sum_{m=1}^M \left[ \sum_{n=1}^N P(\Delta E_m, Y_n) \right],$$

where  $Y$  is any of the  $Y$  axis parameters;

$$\text{Total Deposited Dose} = \frac{C}{M} \sum_{m=1}^M \left[ \sum_{n=1}^N \Delta E_m P(\Delta E_m, Y_n) \right],$$

where  $M$  is the weight of material in the cavity and  $C$  is the constant relating MeV to ergs;

$$\text{Total Deposited Dose Equivalent} = \frac{C}{M} \sum_{m=1}^M \left[ \sum_{n=1}^N (\Delta B)_n P(\Delta E_m, \Delta B_n) \right];$$

$$\text{Event-averaged Quality Factor} = \frac{\sum_{m=1}^M \left[ \sum_{n=1}^N \bar{Q}_n P(\Delta E_m, \bar{Q}_n) \right]}{\text{Number of Events}}$$

$$\left( \frac{dE}{dx} \right) \text{ spectrum, events in } n^{\text{th}} \left( \frac{dE}{dx} \right) \text{ interval} = \sum_{m=1}^M P \left[ \Delta E_m, \left( \frac{dE}{dx} \right)_n \right];$$

$$\text{Deposited dose spectrum, events in } m^{\text{th}} \Delta E \text{ interval} = \sum_{n=1}^N P(\Delta E_m, Y_n);$$

$$\text{Deposited dose distribution, dose in } n^{\text{th}} \left( \frac{dE}{dx} \right) \text{ interval} =$$

$$\frac{C}{M} \sum_{m=1}^M \Delta E_m P \left[ \Delta E_m, \left( \frac{dE}{dx} \right)_n \right].$$



Current running time is about 5 min for a problem consisting of 108,000 cavity events ( $i \times j \times k$ ), shared equally by proton and carbon recoils in both wall and cavity, and involving one Y parameter. A substantial reduction in time could be achieved through more efficient programming.

## VERIFICATION

It is important to determine, first, whether the computer program yields spectral distributions that compare well with both experiment and theory.

To provide experimental check, a series of irradiations were performed at the Argonne 4.5-MeV Van de Graaff accelerator, using the reaction  $\text{Li}^7(p,n)\text{Be}^7$  to produce neutrons up to 1.81 MeV.

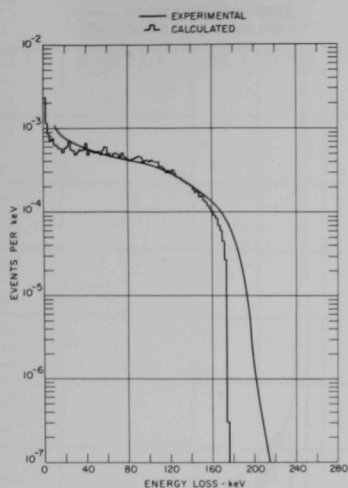
The Rossi LET counter system used has been described elsewhere.<sup>5</sup> The 8-in.-diam chamber was selected on the basis of its superior sensitivity. The fill-gas was a tissue-equivalent mixture at a pressure of 8.8 mm, resulting in a cavity of 2.08- $\mu\text{m}$  effective diameter. Irradiations were made at a 2-m distance from the target to minimize neutron-energy spread, and the background due to secondarily scattered neutrons from the environment were subtracted by making a second run with a paraffin shadow cone interposed between the target and the counter.

Calculations were made with the described computer program, for a cavity having the same physical size and fill pressure, to determine the expected response at the same energies. The calculated and experimental spectra for 500 keV and 1.81 MeV are compared in Figs. 3 and 4. For purposes of comparison, the experimental spectra are normalized to equalize the number of events above 12 keV.

It can be seen that the agreement is quite good at these energies. The most apparent difference is in the end-point energy loss. A linear extrapolation of the end points shows a difference of about seven percent between calculated and experimental curves. This corresponds well with the measured counter resolution of  $6\frac{1}{2}$  percent half-width at half-height. Other shape distortions are probably also due to the counter collection and multiplication characteristics. Significantly, all major characteristics of the curve shape are found to correspond.

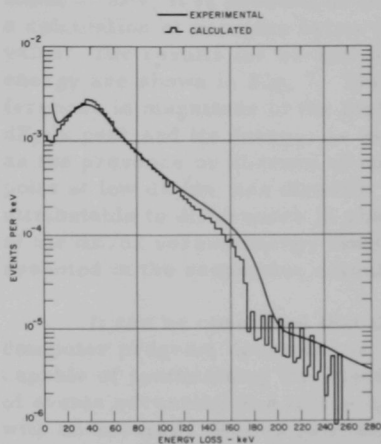
A second test of the calculations is a comparison of the distribution of deposited energy as a function of  $dE/dx$  with that predicted by the theory of Boag.<sup>14</sup> The comparisons made for 2.5- and 14-MeV neutrons using a 0.1- $\mu\text{m}$  cavity are shown in Figs. 5 and 6, respectively. As can be seen, agreement is quite good. Although Boag's expression for  $D\left(\frac{dE}{dx}\right)$  has a





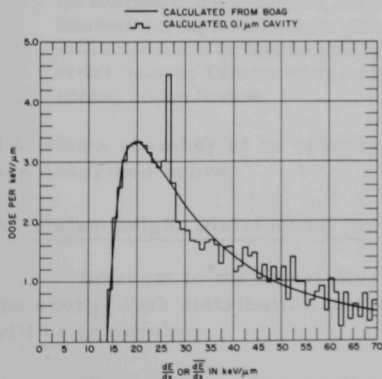
235-1513

Fig. 3. Comparison between Pulse-height Spectrum Obtained Experimentally with 500-keV Neutrons, Using an 8-in. LET Counter, and the Spectrum Calculated with the Described Computer Program. Ordinate values for the calculated spectrum are for unit neutron fluence.



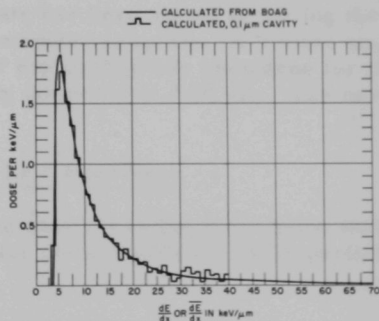
235-1516

Fig. 4. Comparison between Pulse-height Spectrum Obtained Experimentally with 1.81-MeV Neutrons, Using an 8-in. LET Counter, and the Spectrum Calculated with the Described Computer Program. Ordinate values for the calculated spectrum are for unit neutron fluence.



235-1508

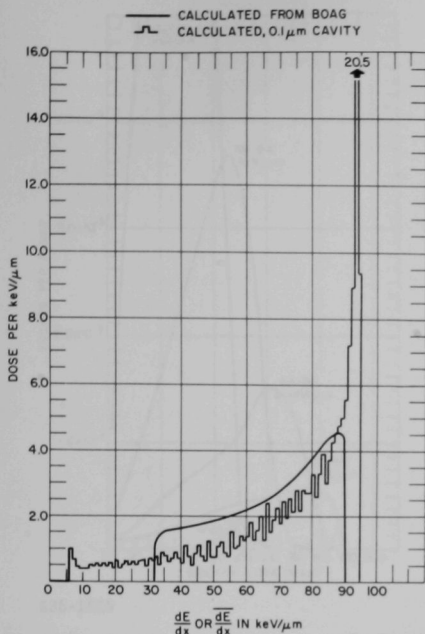
Fig. 5. Comparison between the Distribution of Deposited Energy in  $\overline{dE/dx}$ , as Calculated with the Described Computer Program, and the Distribution of Deposited Energy in  $dE/dx$ , as Calculated from the Boag Equation, for 2.5-MeV Neutrons. Ordinate values are for arbitrary neutron fluences.



235-1510

Fig. 6. Comparison between the Distribution of Deposited Energy in  $\overline{dE/dx}$ , as Calculated with the Described Computer Program, and the Distribution of Deposited Energy in  $dE/dx$ , as Calculated from the Boag Equation, for 14-MeV Neutrons. Ordinate values are for arbitrary neutron fluences.





235-1518

Fig. 7. Comparison between the Distribution of Deposited Energy in  $dE/dx$ , as Calculated with the Described Computer Program, and the Distribution of Deposited Energy in  $dE/dx$ , as Calculated from the Boag Equation for 80-keV Neutrons. Ordinate values are for arbitrary neutron fluences.

8-in.-diam chamber at an effective cavity diameter of  $2.08 \mu\text{m}$ . The results are described below.

#### A. Pulse-height Distribution for Mono-LET Particles

Inherent to the Rossi-Rosenzweig analysis is the assumption that the energy loss distribution in a cavity for mono- $dE/dx$  (or LET) particles will be triangular.

The problem of event distribution has been programmed and run for an 8-in.-diam Rossi chamber filled to 8.8 mm Hg pressure (corresponding to a tissue cavity of  $2.08 \mu\text{m}$ ) and irradiated by isotropic neutron fluences of 2.5 MeV, 500 keV, and 80 keV. The basic output is a three-dimensional display of event probability as a function of energy loss and average  $dE/dx$ , and is difficult to display meaningfully. Figures 8, 9, and 10 show two-dimensional sections of event probability as a function of energy loss in selected  $dE/dx$  intervals for the respective energies.

discontinuity at a proton energy of about 87 keV, it is possible to make a calculation at energies below this value. The results for 80-keV neutron energy are shown in Fig. 7. The differences in magnitude of the high  $dE/dx$  peak and its energy, as well as the presence or absence of cutoff point at low  $dE/dx$ , are directly attributable to differences in shape of the  $dE/dx$  versus energy functions assumed in the respective calculations.

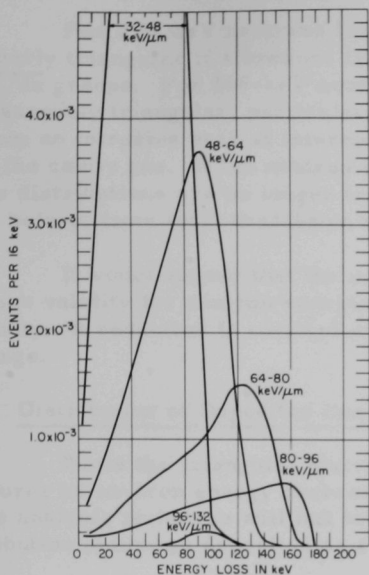
It can be concluded that the computer program described is capable of synthesizing the spectra of events occurring in a tissue cavity with an accuracy limited primarily by choice of the basic  $dE/dx$  versus energy information chosen. It appears also that the accuracy is sufficient for use as a model to explore and test many of the relationships attendant to neutron irradiation of tissue cavities.

## RESULTS

Most of the computations to date has been aimed at testing the computer program. A limited amount of exploration has been done for the

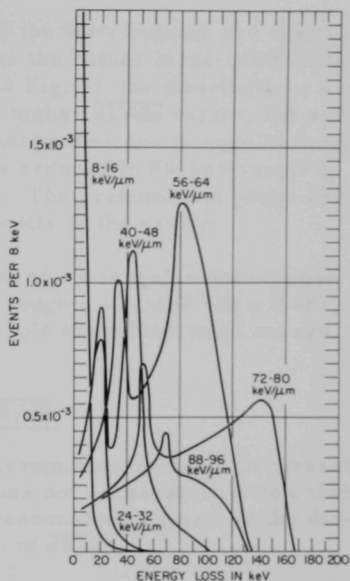






235-1515

Fig. 8. Contribution to the Event Spectrum by Events in the Indicated  $dE/dx$  Groups, as Calculated with the Described Computer Program for 2.5-MeV Neutrons. The ordinate values are for unit neutron fluence.



235-1519

Fig. 9. Contribution to the Event Spectrum by Events in the Indicated  $dE/dx$  Groups, as Calculated with the Described Computer Program for 500-keV Neutrons. The ordinate values are for unit neutron fluence.

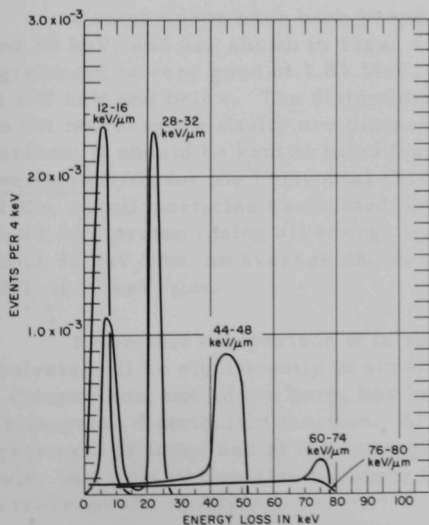


Fig. 10

Contribution to the Event Spectrum by Events in the Indicated  $dE/dx$  Groups, as Calculated with the Described Computer Program for 80-keV Neutrons. The ordinate values are for unit neutron fluence.

235-1511



For 2.5-MeV neutrons (see Fig. 8) the distributions are seen to be clearly triangular if allowance is made for the rather large width of the  $\overline{dE/dx}$  groups. For 500-keV neutrons (see Fig. 9), the distributions are reasonably triangular, particularly at the higher  $\overline{dE/dx}$  values, but suffer from an intrusive peak at intermediate energy loss due to recoils originating in the cavity gas. If the neutron energy is reduced to 80-keV (see Fig. 10), the distributions are no longer triangular. The predominant peaks result, as before, from total absorption of the recoils in the cavity.

It would appear that the assumption of a triangular distribution loses validity for neutron energies below roughly 1.0 MeV for a 2.08- $\mu\text{m}$  cavity. A reduction in cavity diameter should extend the valid energy range.

### B. Distribution of Deposited Energy in $\overline{dE/dx}$

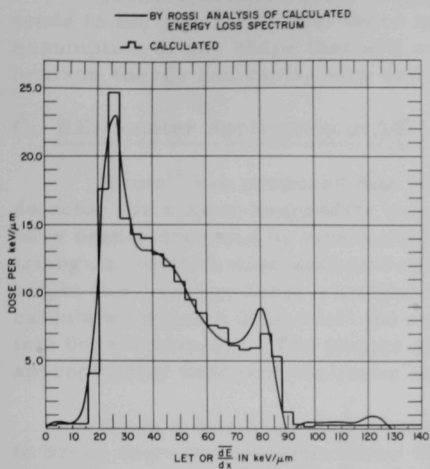
While the triangular distribution assumption becomes progressively poorer as neutron energy decreases, it does not necessarily follow that the analysis technique will fail to give a reasonable estimate of the distribution of energy deposited as a function of  $\overline{dE/dx}$ .

As mentioned earlier, the computer program calculates both the expected pulse-height spectrum and the energy-loss distribution in  $\overline{dE/dx}$ . The pulse-height spectrum can be further analyzed, using the Rossi-Rosenzweig technique, to give the same distribution. From the degree of agreement between the two distributions, we can appraise the validity of the Rossi-Rosenzweig technique.

Comparisons have been prepared for 1.81 MeV, 500 keV, 200 keV, and 80 keV, and are shown in Figs. 11-14, respectively. As can be seen, agreement is very good at 1.81 MeV, adequate at 500 keV, and very poor at 200 keV and below. The distortions that arise in analyzing events that do not traverse the cavity are dramatically apparent in the 80-keV comparison; it should be kept in mind that the theoretical curve uses the average  $dE/dx$  for the horizontal axis, a figure lower than the initial  $dE/dx$  of the recoil particles associated with 80-keV neutrons. For example an 80-keV proton losing all energy in the cavity has an initial  $dE/dx$  of about 93 keV/ $\mu\text{m}$ , an average  $dE/dx$  of 58 keV/ $\mu\text{m}$ , and a Rossi analyzed LET of 39 keV/ $\mu\text{m}$ .

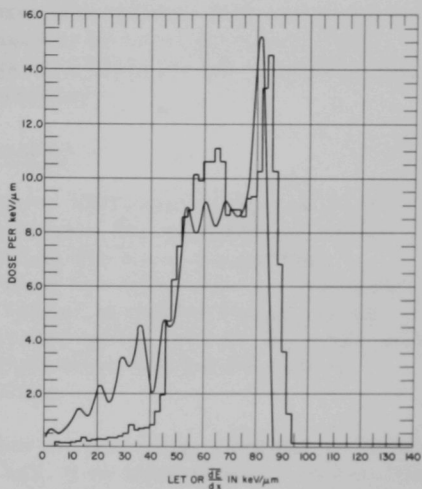
From this comparison it is apparent that the Rossi-Rosenzweig analysis will be significantly in error for neutrons below about 500 keV. A comparison, not shown here, has been made for a square rather than a triangular distribution function. At low energies, a somewhat better agreement is found and at high energies a poorer agreement. Analysis under this assumption also becomes invalid as the recoil particles fail to traverse the cavity.





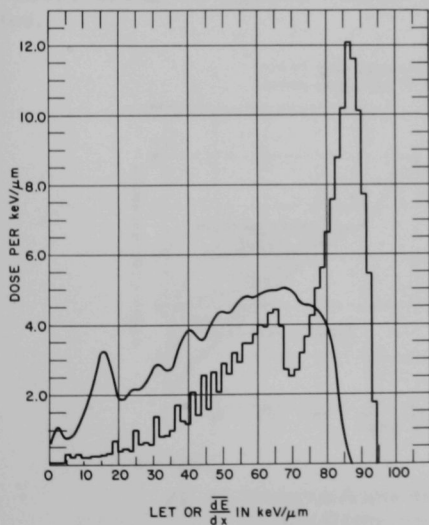
235-1517

Fig. 11. For 1.81-MeV Neutrons



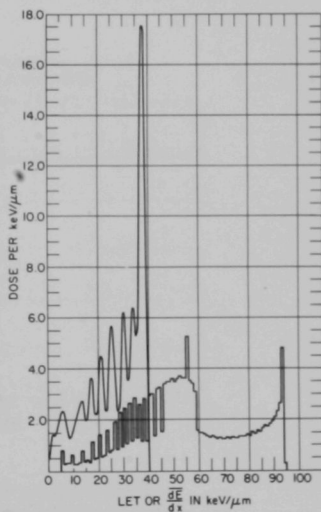
235-1509

Fig. 12. For 500-keV Neutrons



235-1514

Fig. 13. For 200-keV Neutrons



235-1512

Fig. 14. For 80-keV Neutrons

Figs. 11-14. The Energy-loss Spectrum and Dose Distribution in  $dE/dx$  Were Calculated with the Described Computer Program (see individual figure for neutron energy). The energy-loss spectrum was then analyzed by the Rossi technique. Comparison is made between results of the Rossi analysis and the computer calculation. The ordinate values are for arbitrary neutron fluences.

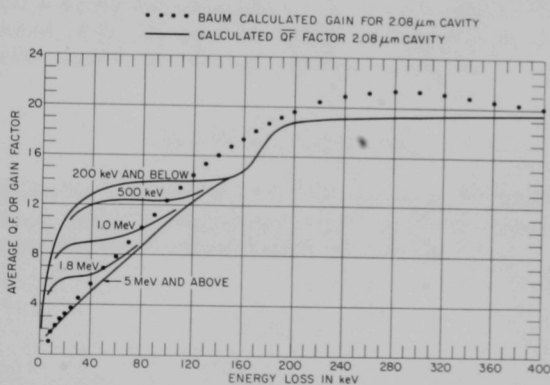


A more detailed study using three-dimensional data presentation leads to the conclusion that there appears to be no single distribution assumption of any shape that will serve as a basis for data analysis unless neutron energy and cavity size are restricted.

### C. REM-meter Application of LET Counter

Baum<sup>15</sup> has proposed that the Rossi LET counter be used as the detector for a Rem-responding survey meter. His calculations, which have been elaborated by Anderson,<sup>16</sup> utilize the Rossi-Rosenzweig triangular-distribution assumption to show that with each value of pulse height (i.e., energy loss) a multiplier related to Quality Factor can be calculated which will convert the integrated energy loss for the spectrum into dose equivalent. The proper multiplication is achieved with an appropriately designed nonlinear amplifier.

Since it has been shown here that the triangular distribution begins to break down for neutrons below 500 keV, it is appropriate to re-examine this concept. A program output that yielded the event-averaged Quality Factor for each energy-loss interval was utilized. Runs were made for a 2.08- $\mu\text{m}$  cavity and for energies between 50 keV and 14 MeV. The results are shown in Fig. 15 together with the Baum calculated multiplication factor.



235-1507

Fig. 15. Comparison Is Made between Quality Factor as a Function of Energy Loss (pulse height) for Various Neutron Energies, and the Gain Factor Proposed for the Baum REM-responding Survey Meter

From this set of curves, it can be seen that for a cavity of this size, the shape of the amplification curve is a function of energy with a limiting envelope for both high and low neutron energies. As would be expected, the Baum curve approximates the high-energy envelope. It is





estimated that the Baum instrument would be in error by about a factor of two for 50-keV monoenergetic neutrons, whereas the error would be negligible for neutrons with energies greater than 2 MeV. It is further estimated that to give negligible error as low as 50 keV, the cavity diameter must be reduced to about 0.2  $\mu\text{m}$ .

## CONCLUSIONS

A computer program has been described for calculating the properties of neutron-initiated events traversing a spherical cavity within a tissue-like medium. Calculated pulse-height distributions correspond well with experimentally produced spectra, and deposited dose versus  $dE/dx$  distributions are in agreement with the predictions of Boag.

Examples are given indicating that the primary limitation of the Rossi-Rosenzweig LET analysis is imposed by the triangular-distribution assumption. Where cavity size is sufficiently small for the neutron energies involved, the assumption is reasonable and the results of the analysis are correct. It is shown that, for a 2.08- $\mu\text{m}$  cavity, the failure point is in the region of neutron energy between 500 and 1000 keV.

It follows that any cavity calculation using the triangular-distribution assumption will also become inaccurate at some lower limit of neutron energy. The case of the Baum Rem-meter is considered, and the extent of expected error in the low-energy region is indicated.

## ACKNOWLEDGMENT

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